Supporting Information for Microfilm Edition

Tables

Table 1. Proton resonance assignments of precursor nisin in aqueous solution at 5°C and pH 3.5.

Residue	NH	αH	βH	Others
Ser-22	–	–[a]	–[a], –[a]	
Thr-21	8.76	4.36	4.20	γCH_3 1.21
Lys-20	8.48	4.23	1.68, 1.68	γCH_2 1.32, 1.32, δCH_2 1.63, 1.63 ϵCH_2 2.92, 2.92, ϵNH_3^+ 7.58
Asp-19	8.37	4.61	2.78, 2.67	
Phe-18	8.29	4.51	3.12, 3.02	2H,6H 7.24, 3H,5H 7.34, 4H –[b]
Asn-17	8.37	4.60	2.77, 2.68	γNH_2 7.67, 6.96
Leu-16	8.19	4.23	1.60, 1.60	γH 1.60, δCH_3 0.93, 0.86
Asp-15	8.43	4.61	2.86, 2.75	
Leu-14	8.12	4.31	1.65, 1.65	γH 1.58, δCH_3 0.93, 0.84
Val-13	8.09	4.08	2.08	γCH_3 0.94, 0.94
Ser-12	8.41	4.45	3.83, 3.83	
Val-11	8.27	4.15	2.11	γCH_3 0.94, 0.94
Ser-10	8.43	4.41	3.94, 3.85	
Lys-9	8.47	4.30	–[b], –[b]	γCH_2 1.43, 1.43, δCH_2 1.66, 1.66 ϵCH_2 2.97, 2.97, ϵNH_3^+ 7.59
Lys-8	8.40	4.25	1.76, 1.76	γCH_2 1.42, 1.42, δCH_2 1.65, 1.65 ϵCH_2 2.97, 2.97, ϵNH_3^+ 7.59
Asp-7	8.53	4.69	2.86, 2.76	
Ser-6	8.43	4.40	3.86, 3.86	
Gly-5	8.52	3.95, 3.95		
Ala-4	8.15	4.34	1.36	
Ser-3	8.44	4.73	3.86, 3.86	
Pro-2	–	4.42	2.29, 1.88	γCH_2 2.01, 2.01, δCH_2 3.83, 3.72
Arg-1	8.44	4.34	1.84, 1.74	γCH_2 1.65, 1.57, δCH_2 3.18, 3.18 NH 7.23, 6.89, 6.50

Residue	NH	αH	βH	Others
Ile1	8.23	4.22	1.96	γCH_2 1.55, 1.25
				γCH_3 1.00, δCH_3 0.88
Dhb2	9.64	–	6.60	γCH_3 1.76
Ala_S3	8.03	4.54	3.24, 3.13	
Ile4	7.78	4.32	2.06	γCH_2 1.34, 1.11
				γCH_3 0.92, δCH_3 0.84
Dha5	9.94	–	5.53, 5.39	
Leu6	9.08	4.42	1.71, 1.71	γH 1.66, δCH_3 0.93, 0.86
$_S$Ala7	8.29	4.44	3.03, 2.93	
Ala^*_S8	8.96	5.08	3.57	γCH_3 1.29
Pro9	–	4.41	2.46, 1.76	γCH_2 2.19, 1.92, δCH_2 3.43, 3.38
Gly10	8.67	4.47, 3.47		
$_S$Ala11	7.83	3.98	3.62, 3.00	
Lys12	8.74	4.28	1.77, 1.77	γCH_2 1.49, 1.35, δCH_2 1.67, 1.67
				ϵCH_2 2.97, 2.97, ϵNH_3^+ 7.59
Ala^*_S13	8.58	4.60	3.62	γCH_3 1.32
Gly14	8.30	4.15, 4.03		
Ala15	8.72	4.18	1.45	
Leu16	8.60	4.32	1.74, 1.74	γH 1.63, δCH_3 0.88, 0.88
Met17	7.79	4.70	2.30, 2.10	γCH_2 2.59, 2.39, ϵCH_3 2.04
Gly18	8.14	4.08, 3.81		
$_S$Ala19	7.68	4.48	2.97, 2.88	
Asn20	8.64	4.65	2.79, 2.79	γNH_2 7.67, 6.99
Met21	8.40	4.49	2.12, 1.99	γCH_2 2.59, 2.50, ϵCH_3 2.08
Lys22	8.52	4.28	1.83, 1.83	γCH_2 1.47, 1.42, δCH_2 1.69, 1.69
				ϵCH_2 2.97, 2.97, ϵNH_3^+ 7.59
Ala^*_S23	8.95	4.96	3.53	γCH_3 1.33
Ala24	8.28	4.63	1.43	
Ala^*_S25	9.27	4.76	3.51	γCH_3 1.44
$_S$Ala26	7.85	3.83	3.40, 2.65	
His27	8.81	4.89	3.34, 3.04	2H 8.61, 4H 7.30
$_S$Ala28	7.98	4.40	3.67, 2.66	
Ser29	8.54	4.45	3.83, 3.83	

Residue	NH	αH	βH	Others
Ile30	8.27	4.16	1.81	γCH_2 1.34, 1.14
				γCH_3 0.84, δCH_3 0.84
His31	8.75	4.75	3.21, 3.15	2H 8.58, 4H 7.25
Val32	8.43	4.14	2.05	γCH_3 0.94, 0.94
Dha33	9.79	–	5.68, 5.68	
Lys34	8.33	4.26	1.88, 1.77	γCH_2 $-^b$, $-^b$, δCH_2 1.66, 1.66
				ϵCH_2 2.97, 2.97, ϵNH_3^+ 7.59

[a]Resonance could not be identified.

[b]Overlap of resonances.

Table 2. Proton resonance assignments of precursor nisin complexed to DPC micelles at 40°C and pH 3.5.

Residue	NH	αH	βH	Others
Ser-22	–	–[a]	–[a], –[a]	
Thr-21	8.68	4.30	4.21	γCH_3 1.20
Lys-20	8.25	4.24	1.70, 1.70	γCH_2 1.52, 1.37, δCH_2 1.65, 1.65 ϵCH_2 2.96, 2.96, ϵNH_3^+ 7.51
Asp-19	8.18	4.70	2.75, 2.75	
Phe-18	8.04	4.48	3.08, 3.02	2H,6H 7.20, 3H,5H 7.24, 4H 7.16
Asn-17	8.15	4.70	2.78, 2.72	γNH_2 7.52, 6.75
Leu-16	8.10	4.19	1.65, 1.65	γH 1.58, δCH_3 0.92, 0.85
Asp-15	8.31	4.68	2.84, 2.84	
Leu-14	8.05	4.16	1.67, 1.67	γH 1.58, δCH_3 0.91, 0.84
Val-13	7.75	3.94	2.17	γCH_3 0.98, 0.92
Ser-12	7.98	4.36	3.86, 3.86	
Val-11	7.90	4.02	2.16	γCH_3 0.95, 0.95
Ser-10	8.06	4.34	3.91, 3.85	
Lys-9	8.02	4.24	1.86, 1.79	γCH_2 1.48, 1.42 , δCH_2 –[b], –[b] ϵCH_2 2.96, 2.96, ϵNH_3^+ 7.51
Lys-8	8.01	4.23	1.80, 1.80	γCH_2 1.43, 1.43, δCH_2 1.65, 1.65 ϵCH_2 2.96, 2.96 , ϵNH_3^+ 7.51
Asp-7	8.18	4.71	2.88, 2.76	
Ser-6	8.04	4.35	3.92, 3.85	
Gly-5	8.33	3.93, 3.93		
Ala-4	7.90	4.34	1.34	
Ser-3	8.13	–[a]	3.85, 3.85	
Pro-2	–	4.39	2.21, 1.84	γCH_2 1.95, 1.95, δCH_2 3.77, 3.77
Arg-1	8.30	4.37	1.85, 1.81	γCH_2 1.70, 1.66 , δCH_2 3.20, 3.20 NH 7.51, –[a]
Ile1	8.13	4.08	2.04	γCH_2 1.58, 1.23 γCH_3 0.96, δCH_3 0.85
Dhb2	9.20	–	6.53	γCH_3 1.75
Ala_S3	–[a]	–[a]	–[a], –[a]	

Residue	NH	αH	βH	Others
Ile4	8.15	3.92	1.94	γCH_2 1.46, 1.25
				γCH_3 0.92, δCH_3 0.83
Dha5	8.65	–	6.22, 5.56	
Leu6	9.09	4.00	1.78, 1.78	γH 1.60, δCH_3 0.89, 0.89
$_S$Ala7	–[a]	–[a]	–[a], –[a]	
Ala$^*_S$8	8.85	5.03	3.53	γCH_3 1.24
Pro9	–	4.42	2.33, 1.71	γCH_2 2.00, 2.00, δCH_2 3.57, 3.42
Gly10	–[a]	–[a], –[a]		
$_S$Ala11	7.88	3.98	3.61, 2.98	
Lys12	8.38	4.30	1.76, 1.76	γCH_2 1.46, 1.34, δCH_2 1.66, 1.66
				ϵCH_2 2.96, 2.96, ϵNH_3^+ 7.51
Ala$^*_S$13	8.21	–[a]	3.60	γCH_3 1.28
Gly14	8.21	4.00, –[a]		
Ala15	8.73	4.18	1.41	
Leu16	8.49	4.18	1.73, 1.73	γH 1.64, δCH_3 0.87, 0.87
Met17	7.60	4.61	2.25, 2.06	γCH_2 2.61, 2.41, ϵCH_3 2.04/2.06[c]
Gly18	7.98	4.06, 3.76		
$_S$Ala19	7.57	4.40	2.94, 2.89	
Asn20	8.39	4.58	2.82, 2.76	γNH_2 7.55, 6.83
Met21	8.23	4.45	2.11, 1.96	γCH_2 2.56, 2.47, ϵCH_3 2.04/2.06[c]
Lys22	8.12	4.21	1.80, 1.80	γCH_2 1.47, 1.40, δCH_2 1.67, 1.67
				ϵCH_2 2.96, 2.96, ϵNH_3^+ 7.51
Ala$^*_S$23	8.72	4.93	3.50	γCH_3 1.30
Ala24	8.19	4.66	1.40	
Ala$^*_S$25	9.10	4.74	3.47	γCH_3 1.37
$_S$Ala26	7.75	3.79	3.38, 2.63	
His27	8.70	4.88	3.36, 3.03	2H 8.59, 4H 7.28
$_S$Ala28	7.70	4.35	3.58, 2.68	
Ser29	8.51	4.43	3.79, 3.79	
Ile30	7.85	4.20	1.79	γCH_2 1.36, 1.10
				γCH_3 0.82, δCH_3 0.82
His31	8.46	4.78	3.23, 3.10	2H 8.55, 4H 7.23
Val32	8.25	4.13	2.10	γCH_3 0.91, 0.91

Residue	NH	αH	βH	Others
Dha33	9.21	–	5.94, 5.74	
Lys34	8.16	4.29	1.88, 1.79	γCH_2 1.45, 1.45, δCH_2 1.68, 1.68
				ϵCH_2 2.96, 2.96, ϵNH_3^+ 7.51

[a]Resonance could not be identified.

[b]Overlap of resonances.

[c]It was not possible to assign the methyl groups to the individual methionines.